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=> d que
L1                STR
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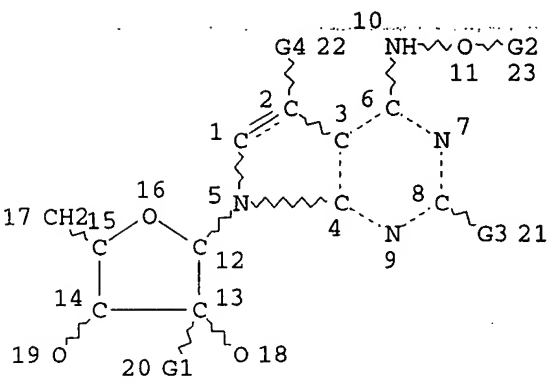

Ak @24

S Ak
@25 26

O C Ak
27 @28 29

O C O
@30 31 32

O C N
33 @34 35

HO B OH
36 @37 38

G5 N C G6
39 40 @41 42

Ak @43

O Ak
@44 45

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VAR G1=H/AK
VAR G2=H/24
VAR G3=H/X/OH/25/N
VAR G4=28/30/CN/COOH/X/34/37/41/NO2/43
VAR G5=H/OH/N/44
VAR G6=H/AK/N
NODE ATTRIBUTES:
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CONNECT  IS E1  RC AT  24
CONNECT  IS E1  RC AT  26
CONNECT  IS E1  RC AT  29
DEFAULT MLEVEL IS ATOM
GGCAT    IS LOC  AT  24
GGCAT    IS UNS  AT  43
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  45

STEREO ATTRIBUTES: NONE
L3            17 SEA FILE=REGISTRY SSS FUL L1
L4             5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L9             6 SEA FILE=MARPAT SSS FUL L1
L10            4 SEA FILE=MARPAT ABB=ON  PLU=ON  L9 NOT L4


=> d l10 ibib abs qhit 1-4

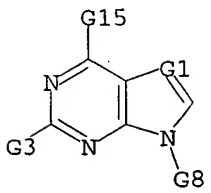
L10  ANSWER 1 OF 4  MARPAT  COPYRIGHT 2005 ACS on STN
```

ACCESSION NUMBER: 138:379194 MARPAT
TITLE: Ribonucleoside analogs for inhibition of RNA viruses
INVENTOR(S): Loakes, David; Brown, Daniel; Balzarini, Jan; Moriyama, Kei; Negishi, Kazuo; Cameron, Craig; Arnold, Jamie; Castro, Christian; Korneeva, Victoria; Graci, Jason
PATENT ASSIGNEE(S): Medical Research Council, UK
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

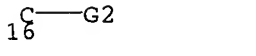
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003039450	A2	20030515	WO 2002-GB5031	20021107
WO 2003039450	A3	20030821		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003130226	A1	20030710	US 2002-207005	20020730
EP 1441744	A2	20040804	EP 2002-772630	20021107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005507944	T2	20050324	JP 2003-541742	20021107
PRIORITY APPLN. INFO.:			GB 2001-26701	20011107
			US 2002-207005	20020730
			WO 2002-GB5031	20021107

AB The invention discloses pharmaceutical compns. containing ribonucleoside analogs, in admixt. with a physiol. acceptable excipient diluent or carrier. The ribonucleoside analogs of the invention inhibit the replication and/or increase the mutation rate of an RNA virus. Preparation of analogs is described. The compds. may be used to treat viral infections in animals, including humans, and plants.

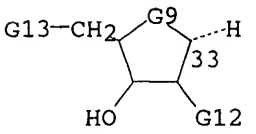
MSTR 1



G1 = 16



G2 = acyl
G8 = 33



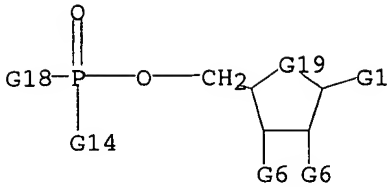
G9 = O
G12 = OH
G16 = NH
G18 = OH
MPL: claim 1

L10 ANSWER 2 OF 4 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 131:267028 MARPAT
TITLE: Nucleosides with antiviral and anticancer activity, and preparation thereof
INVENTOR(S): Wagner, Carston R.; Griesgraber, George W.
PATENT ASSIGNEE(S): Regents of the University of Minnesota, USA
SOURCE: PCT Int. Appl., 91 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

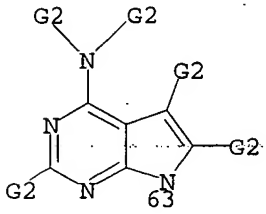
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9949873	A1	19991007	WO 1999-US6467	19990326
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2326535	AA	19991007	CA 1999-2326535	19990326
AU 9933634	A1	19991018	AU 1999-33634	19990326
US 6475985	B1	20021105	US 2000-647206	20000927
PRIORITY APPLN. INFO.:			US 1998-79570P	19980327
			WO 1999-US6467	19990326

AB The invention provides nucleoside derivs. (Markush included) which possess antiviral and anticancer activity. Treatment of breast cancer is a preferred embodiment. Preparation and activity of e.g. 3-azido-3-deoxythymidine-5-methoxy-L-tryptophanyl phosphoramidate is included.

MSTR 1

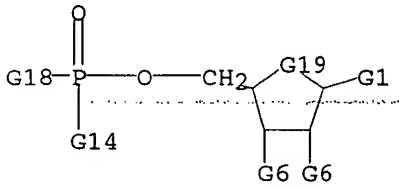


G1 = 63

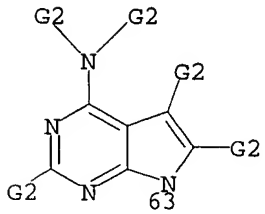


G2 = OH / OCHO
G6 = OH
G19 = O
DER: or pharmaceutically acceptable salts
MPL: claim 1
NTE: also incorporates claim 96
NTE: substitution is restricted

MSTR 2



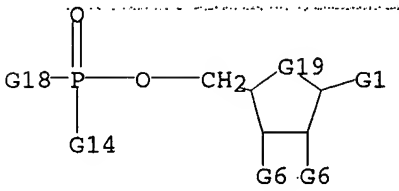
G1 = 63



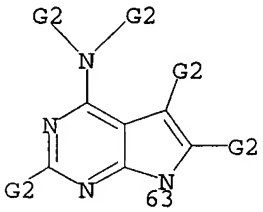
G2 = OH / OCHO
G6 = OH
G19 = O
DER: or pharmaceutically acceptable salts
MPL: claim 53

NTE: also incorporates claim 95
NTE: substitution is restricted

MSTR 3



G1 = 63



G2 = OH / OCHO
G6 = (1-2) OH
G19 = O
DER: or pharmaceutically acceptable salts
MPL: claim 75
NTE: also incorporates claim 97
NTE: substitution is restricted

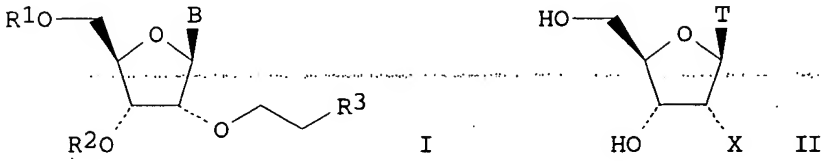
L10 ANSWER 3 OF 4 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 124:146751 MARPAT
TITLE: Preparation of nucleosides and oligonucleotides containing 2'-ether groups as drugs and diagnostic agents.
INVENTOR(S): Martin, Pierre
PATENT ASSIGNEE(S): Ciba-Geigy AG, Switz.; Novartis AG; Novartis Pharma GmbH
SOURCE: Eur. Pat. Appl., 31 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 679657	A2	19951102	EP 1995-810259	19950419
EP 679657	A3	19960410		
EP 679657	B1	20030709		
R: AT, BE, CH, DE, DK, ES, FR, GB, IE, IT, LI, LU, NL, PT, SE				
AT 244723	E	20030715	AT 1995-810259	19950419

PT 679657	T	20031128	PT 1995-810259	19950419
ES 2203635	T3	20040416	ES 1995-810259	19950419
US 5750673	A	19980512	US 1995-426807	19950420
CA 2147798	AA	19951028	CA 1995-2147798	19950425
ZA 9503383	A	19951027	ZA 1995-3383	19950426
AU 9517653	A1	19951102	AU 1995-17653	19950426
AU 682576	B2	19971009		
JP 07300493	A2	19951114	JP 1995-102074	19950426
CN 1115320	A	19960124	CN 1995-104242	19950426
CN 1066456	B	20010530		
US 5977332	A	19991102	US 1998-26713	19980220

PRIORITY APPLN. INFO.: CH 1994-1307 19940427
US 1995-426807 19950420

GI

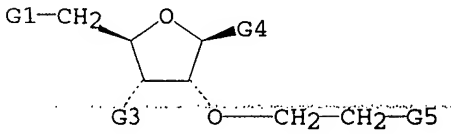


I

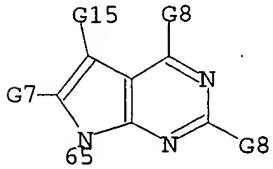
II

AB Title compds. [I; R1 = H, protecting group; R2 = R1, P-containing nucleotide bridging group; B = purine or pyrimidine (analog) residue; R3 = OH, F, (CF2)nCF3; n = 0-7], and oligonucleotides containing them, were prepared as drugs and diagnostic agents. Thus, antisense oligonucleotides TTTTtCTCTCTCTCT t = residue of (II; X = H, OCH2CH2OH, OCH2CH2F, OCH2CH2CF3, OCH2CH2Me) showed ΔTm = 0 to +1.7°.

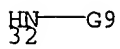
MSTR 1



G3 = OH
G4 = 65



G8 = 32



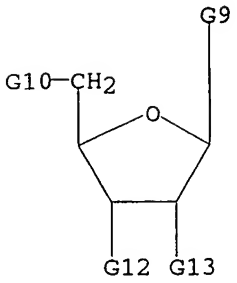
G9 = OH
G15 = CN
MPL: claim 1

L10 ANSWER 4 OF 4 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 119:197257 MARPAT
TITLE: Applications of fluorescent N-nucleosides and fluorescent structural analogs of N-nucleosides
INVENTOR(S): Conrad, Michael J.
PATENT ASSIGNEE(S): Chromagen, Inc., USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

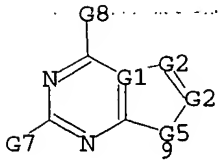
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9316094	A2	19930819	WO 1993-US1338	19930212
WO 9316094	A3	19930930		
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 628051	A1	19941214	EP 1993-905954	19930212
EP 628051	B1	20030702		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07504087	T2	19950511	JP 1993-514326	19930212
AT 244259	E	20030715	AT 1993-905954	19930212
US 5763167	A	19980609	US 1994-214994	19940321
PRIORITY APPLN. INFO.:			US 1992-834456	19920212
			WO 1993-US1338	19930212

AB Analogs of nucleic acid bases that are fluorescent under physiol. conditions are identified for use in fluorescent hybridization probes and methods of synthesis of these analogs are described. These analogs can be incorporated into oligonucleotides by standard chemical or enzymically and are capable of forming Watson-Crick base pairs. The chemical conversion of formycin A to 2'-deoxyformycin A, its phosphorylation to the triphosphate and the preparation of the phosphoramidite are described. Formycin A triphosphate and the 2'-deoxy analog successfully substituted ATP and dATP in the enzymic synthesis of high mol. weight probes from a variety of DNA templates. Probes containing formycin A moieties hybridized successfully and the hybrids showed a stability comparable to those from unsubstituted probes; fluorescence properties were as expected. The use of such probes to detect a number of sequences was demonstrated.

MSTR 1

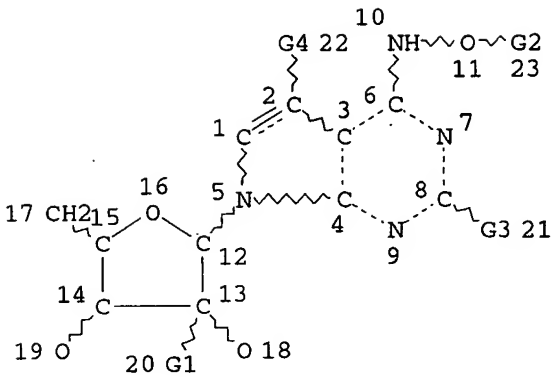


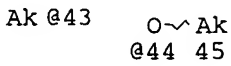
G1 = C
G3 = C
G4 = CN
G5 = N
G8 = NHOH
G9 = 9



G12 = OH
G13 = OH
DER: or structural analogs
MPL: claim 1

=> d que 14
L1 STR





VAR G1=H/AK
VAR G2=H/24
VAR G3=H/X/OH/25/N
VAR G4=28/30/CN/COOH/X/34/37/41/NO2/43
VAR G5=H/OH/N/44
VAR G6=H/AK/N
NODE ATTRIBUTES:
NSPEC IS RC AT 35
CONNECT IS E1 RC AT 24
CONNECT IS E1 RC AT 26
CONNECT IS E1 RC AT 29
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC AT 24
GGCAT IS UNS AT 43
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 45

STEREO ATTRIBUTES: NONE
L3 17 SEA FILE=REGISTRY SSS FUL L1
L4 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=> d l4 ibib abs hitstr 1-5

L4 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:290484 HCAPLUS
DOCUMENT NUMBER: 140:327061

TITLE: Nucleoside derivatives for treating hepatitis C virus infection

INVENTOR(S): Roberts, Christopher Don; Dyatkina, Natalia B.

PATENT ASSIGNEE(S): Genelabs Technologies, Inc., USA

SOURCE: PCT Int. Appl., 119 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004028481	A2	20040408	WO 2003-US31433	20030930
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004147464	A1	20040729	US 2003-676956	20030930
PRIORITY APPLN. INFO.:			US 2002-415222P P	20020930
			US 2003-443169P P	20030129

OTHER SOURCE(S): MARPAT 140:327061

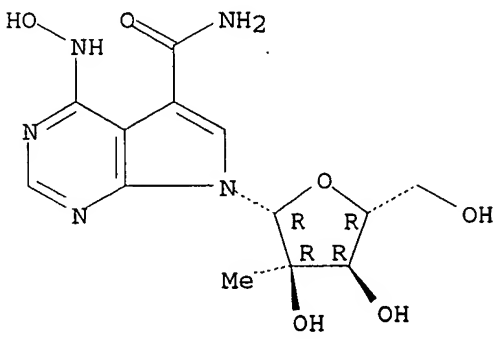
AB Nucleoside compns. and methods for treating hepatitis C virus infections. Thus, 9-(2'-C-methyl-β-D-ribofuranosyl)-6-methoxyaminopurine was prepared by the reaction of 6-chloro-9-(2'-C-methyl-β-D-ribofuranosyl)purine and methxylamine. This compound exhibited anti-hepatitis C activity by inhibiting HCV polymerase.

IT **565455-26-7P 677298-84-9P 677298-85-0P**
677298-90-7P 677298-92-9P 677298-94-1P
677298-95-2P 677299-07-9P 677299-11-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(nucleoside derivs. for treating hepatitis C virus infection)

RN 565455-26-7 HCAPLUS

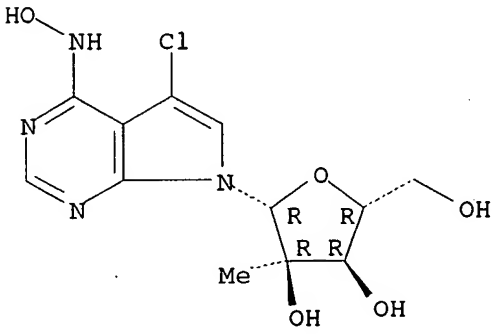
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxamide, 4-(hydroxyamino)-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



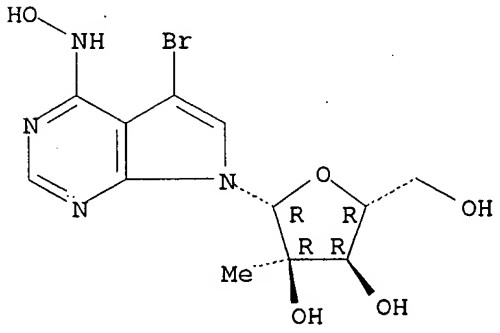
RN 677298-84-9 HCAPLUS
CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 5-chloro-1,7-dihydro-7-(2-C-methyl-β-D-ribofuranosyl)-, oxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.



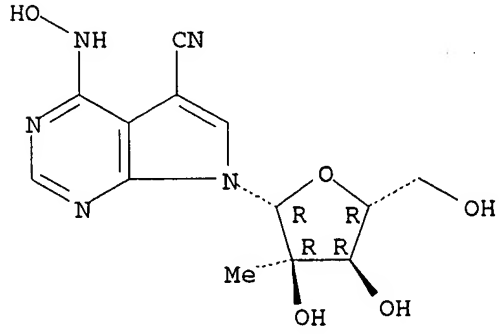
RN 677298-85-0 HCAPLUS
CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 5-bromo-1,7-dihydro-7-(2-C-methyl-β-D-ribofuranosyl)-, oxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.



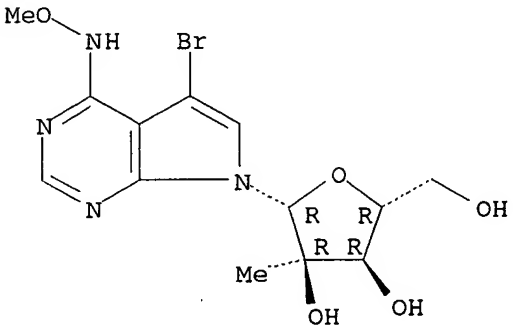
RN 677298-90-7 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carbonitrile, 4-(hydroxyamino)-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



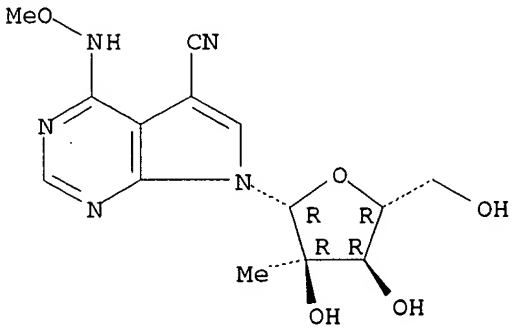
RN 677298-92-9 HCAPLUS
CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 5-bromo-1,7-dihydro-7-(2-C-methyl-β-D-ribofuranosyl)-, O-methyloxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.



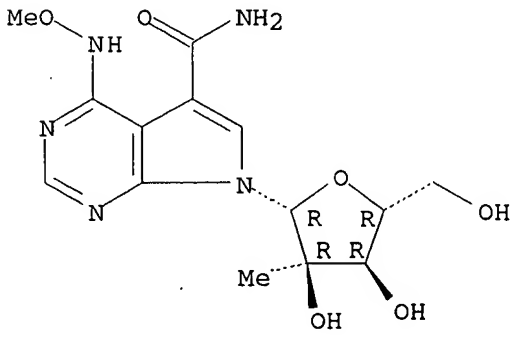
RN 677298-94-1 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carbonitrile, 4-(methoxyamino)-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



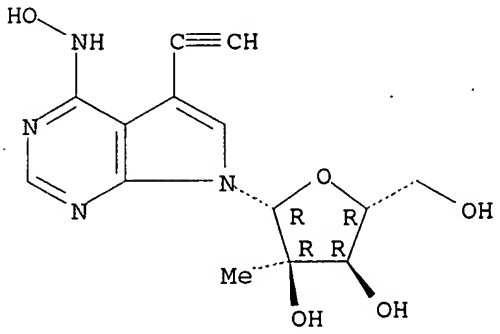
RN 677298-95-2 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxamide, 4-(methoxyamino)-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



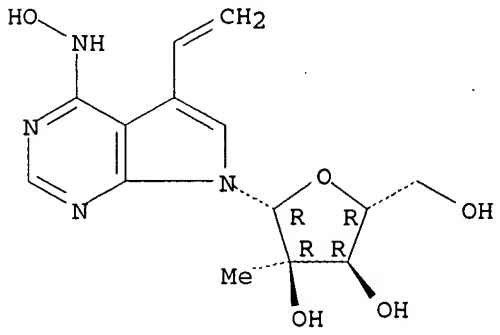
RN 677299-07-9 HCAPLUS
CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 5-ethynyl-1,7-dihydro-7-(2-C-methyl-β-D-ribofuranosyl)-, oxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 677299-11-5 HCAPLUS
CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 5-ethenyl-1,7-dihydro-7-(2-C-methyl-β-D-ribofuranosyl)-, oxime (9CI) (CA INDEX NAME)

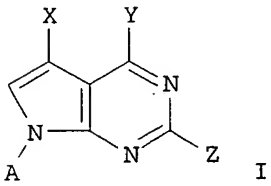
Absolute stereochemistry.



L4 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:590940 HCAPLUS
DOCUMENT NUMBER: 139:133787
TITLE: Preparation of deazapurine nucleoside analogs as antiviral agents
INVENTOR(S): An, Haoyun; Ding, Yili; Chamakura, Varaprasad; Hong, Zhi
PATENT ASSIGNEE(S): Ribapharm Inc., USA
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2003061576 A2 20030731 WO 2003-US1545 20030117
WO 2003061576 A3 20040401
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 2002-350296P P 20020117
OTHER SOURCE(S): MARPAT 139:133787
GI



I

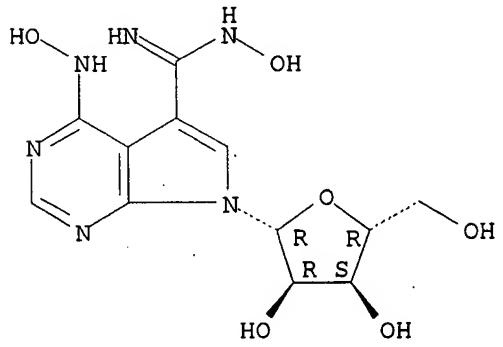
AB Methods, compns., and uses for various deazapurine nucleoside libraries and library compds. I are provided. Particularly preferred deazapurine nucleosides include 7-deazapurine nucleosides, 7-deaza-8-azapurine nucleosides, toyocamycin nucleoside analogs, 3-deazapurine nucleosides, and 9-deazapurine nucleosides, while preferred uses especially include use of such compds. as pharmacol., and particularly antiviral agents. 4-N,N-dimethylamino-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine-5-N-hydroxycarbamidine was prepared and tested in vitro as antiviral agent.

IT **565455-11-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of deazapurine nucleoside analogs as antiviral agents)

RN 565455-11-0 HCAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboximidamide, N-hydroxy-4-(hydroxyamino)-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

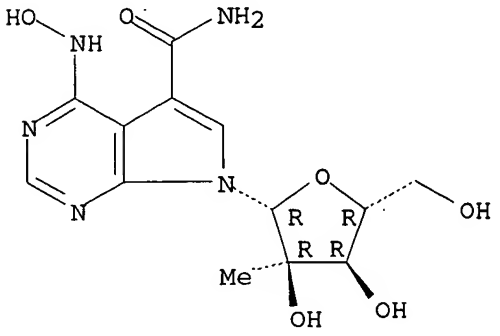
Absolute stereochemistry.



IT **565455-26-7 565455-27-8 565455-28-9**
565455-29-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of deazapurine nucleoside analogs as antiviral agents)

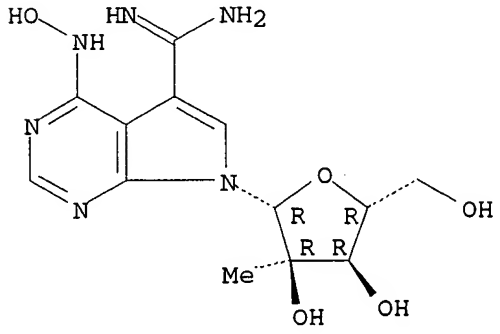
RN 565455-26-7 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxamide, 4-(hydroxyamino)-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



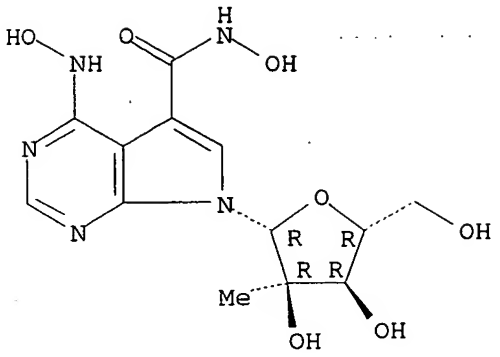
RN 565455-27-8 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboximidamide, 4-(hydroxyamino)-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



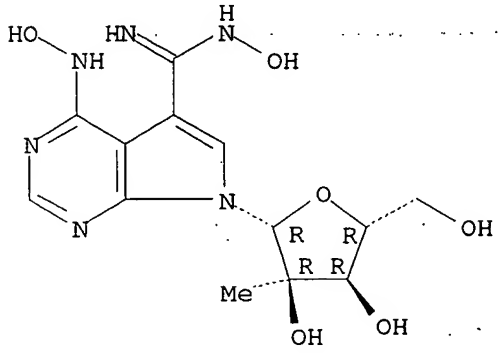
RN 565455-28-9 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxamide, N-hydroxy-4-(hydroxyamino)-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 565455-29-0 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboximidamide, N-hydroxy-4-(hydroxyamino)-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:590191 HCAPLUS
DOCUMENT NUMBER: 123:52110
TITLE: Structure-activity relationship for the binding of nucleoside ligands to adenosine kinase from Toxoplasma gondii
AUTHOR(S): Iltzsch, Max H.; Uber, Sheri S.; Tankersley, Kevin O.; el Kouni, Mahmoud H.
CORPORATE SOURCE: Dept. Biol. Sci., Univ. Cincinnati, Cincinnati, OH, 45221, USA
SOURCE: Biochemical Pharmacology (1995), 49(10), 1501-12
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB One hundred and twenty-eight purine nucleoside analogs were evaluated as ligands of Toxoplasma gondii adenosine kinase (EC 2.7.1.20) by examining their ability to inhibit this enzyme in vitro. Inhibition was quantified by determining apparent Ki (appKi) values for those compds. that inhibited this enzyme by greater than 10% at a concentration of 1 mM. Two compds., N6-(p-methoxybenzoyl)adenosine and 7-iodo-7-deazaadenosine (iodotubercidin), were found to bind to the enzyme (appKi = 3.9 and 1.6 μM, resp.) better than adenosine. On the basis of these data, a

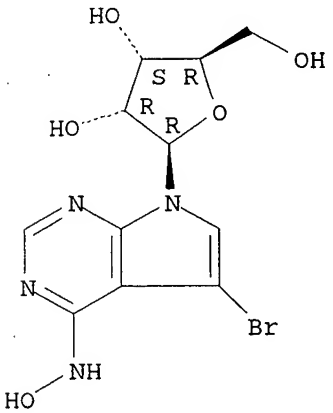
AD 950036

structure-activity relationship for the binding of ligands to T. gondii adenosine kinase was formulated using adenosine as a reference compound It was concluded that the following structures features of purine nucleoside analogs are required or strongly preferred for binding: (1) "pyridine-type" endocyclic nitrogens at the 1- and 3-positions; (2) an exocyclic hydrogen at the 2-position; (3) 6-position exocyclic substituents in the lactim tautomeric form; (4) a "pyridine-type" endocyclic nitrogen at the 7-position or hydrophobic exocyclic substituents attached to an endocyclic carbon at the 7-position; (5) an endocyclic methine or "pyridine-type" nitrogen at the 8-position; (6) an endocyclic nitrogen at the 9-position; (7) a pentose or "pentose-like" (e.g. hydroxylated cyclopentene) moiety attached to the 9-position nitrogen; (8) hydroxyl groups at the 2'- and 3'-positions in a ribose configuration; (9) a hydroxymethyl or Me (i.e. 5'-deoxy) group at the 5'-position; (10) a β-D-nucleoside configuration; and (11) an anti conformation around the N-glycosidic bond. In addition, there appears to be a "pocket" in the catalytic site of T. gondii adenosine kinase, adjacent to the 6-position of adenosine, that can accommodate large (preferably unsatd. or aromatic) substituents (e.g. phenyl). These findings provide the basis for the rational design of addnl. ligands of T. gondii adenosine kinase.

IT **24386-87-6**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(structure-activity relationship for the binding of nucleoside ligands to adenosine kinase from Toxoplasma gondii)

RN 24386-87-6 HCAPLUS
CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 5-bromo-1,7-dihydro-7-β-D-ribofuranosyl-, oxime (9CI) (CA INDEX NAME)

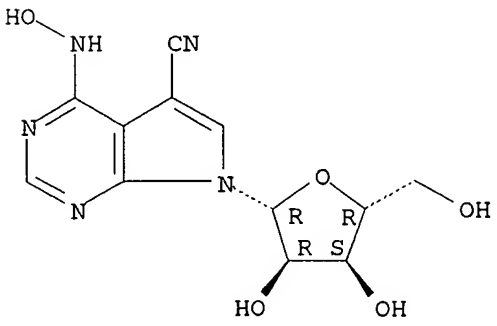
Absolute stereochemistry.



L4 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1975:514793 HCAPLUS
DOCUMENT NUMBER: 83:114793
TITLE: Pyrrolopyrimidine nucleosides. X. Synthesis of 4,5-disubstituted 7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidines related to toyocamycin and sangivamycin
AUTHOR(S): Hinshaw, Barbara C.; Leonoudakis, Olga; Schram, Karl

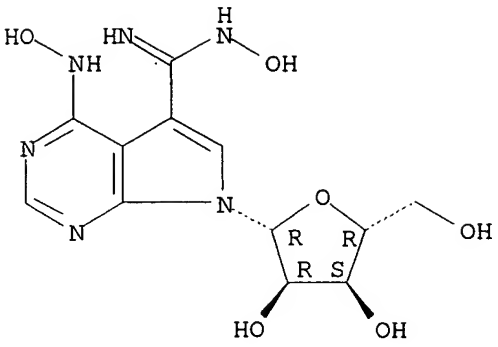
H.; Townsend, Leroy B.
CORPORATE SOURCE: Dep. Biopharm. Sci., Univ. Utah, Salt Lake City, UT, USA
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1975), (13), 1248-53
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The pyrrolopyrimidine I (R = CN, R1 = Cl), prepared from deaminotoyocamycin (II) in 3 steps, with amines gave the corresponding 4-amino derivative E.g., I with MeNH2 gave 67% I (R = CN, R1 = NHMe) which with H2S gave the thiocarboxamide I (R = CSNH2, R1 = NHMe). Other 4-amino derivs. reacted similarly. Catalytic dechlorination of I (R = CN, R1 = Cl) gave the parent carbonitrile I (R = CN, R1 = H) which was compared to II and toyocamycin (III). The CN group of I (R = CN, R1 = H) was more reactive under both basic and acidic conditions than that of II or III, and with NH4OH, NH2OH, and H2S gave I [R = CONH2, C(NH)2:NOH, C(NH2):S, R1 = H], resp.
IT **57071-72-4P 57071-83-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57071-72-4 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carbonitrile, 4-(hydroxyamino)-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 57071-83-7 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboximidamide, N-hydroxy-4-(hydroxyamino)-7-β-D-ribofuranosyl-, monohydrochloride (9CI) (CA INDEX NAME)

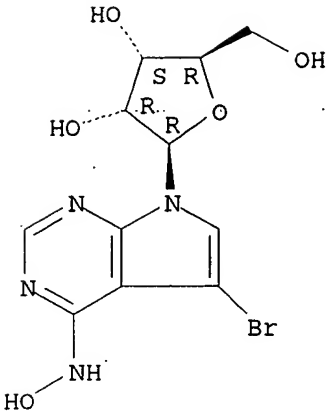
Absolute stereochemistry.



● HCl

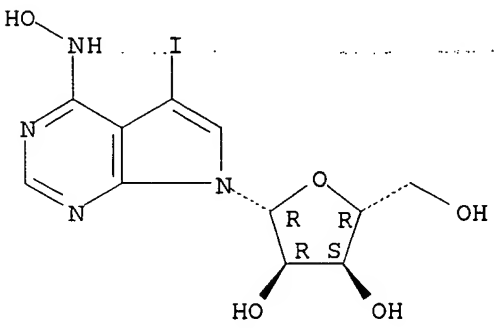
L4 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:413309 HCAPLUS
DOCUMENT NUMBER: 71:13309
TITLE: Pyrrolopyrimidine nucleosides. IV. Synthesis of certain 4,5-disubstituted-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidines related to the pyrrolo[2,3-d]pyrimidine nucleoside antibiotics
AUTHOR(S): Hinshaw, Barbara C.; Gerster, John F.; Robins, Roland K.; Townsend, Leroy B.
CORPORATE SOURCE: Univ. of Utah, Salt Lake City, UT, USA
SOURCE: Journal of Heterocyclic Chemistry (1969), 6(2), 215-21
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The treatment of 4-chloro-7-(2',3',5'-tri-O-acetyl-β-D-ribofuranosyl)pyrrolo[2, 3-d]pyrimidine (I) with N-bromoacetamide in CH2Cl2 furnished the 5-bromo derivative of I which on subsequent deacetylation provided a good yield of 5-bromo-4-chloro-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine (II). Assignment of the halogen substituent to position 5 was made on the basis of 1H N.M.R. studies. Treatment of II with methanolic ammonia afforded 4-amino-5-bromo-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine (5-bromotubercidin) and a subsequent study revealed that the 4-chloro group of II was replaced preferentially in a series of nucleophilic displacement reactions. The analogous synthesis of 4,5-dichloro-7-(β-D-ribofuranosyl)pyrrolo]2, 3-d]-pyrimidine (III) and 4-chloro-5-iodo-7-(β-D-ribofuranosyl)pyrrolo-[2,3-d]pyrimidine (IV) from I furnished 5-chlorotubercidin and 5-iodotubercidin, resp., on treatment of IV and III with methanolic NH3. The possible biochem. significance of these tubercidin derivs. is discussed.
IT **24386-87-6P 24386-92-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24386-87-6 HCAPLUS
CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 5-bromo-1,7-dihydro-7-β-D-ribofuranosyl-, oxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 24386-92-3 HCAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-(hydroxyamino)-5-iodo-7-β-D-ribofuranosyl- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



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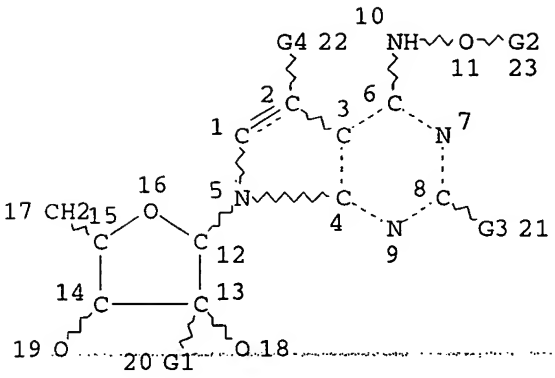
L1 STR



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G5 N C G6
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Ak @43

O Ak
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VAR G2=H/24
VAR G3=H/X/OH/25/N
VAR G4=28/30/CN/COOH/X/34/37/41/NO2/43
VAR G5=H/OH/N/44
VAR G6=H/AK/N
NODE ATTRIBUTES:
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CONNECT IS E1 RC AT 24
CONNECT IS E1 RC AT 26
CONNECT IS E1 RC AT 29
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC AT 24
GGCAT IS UNS AT 43
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 45

STEREO ATTRIBUTES: NONE
L12 3 SEA FILE=BEILSTEIN SSS FUL L1

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L12 ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): 4072006

Beilstein Pref. RN (BPR):	57071-83-7
CAS Reg. No. (RN):	57071-83-7
Fragm. Molec. Formula (FMF):	C12 H16 N6 O6 , Cl H
Molecular Formula (MF):	C12 H16 N6 O6 . Cl H
Molecular Weight (MW):	340.30, 36.46
Fragment BRN (FBRN):	4014421, 1098214
Lawson Number (LN):	30360, 20554
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	3670744
Tautomer ID (TAUTID):	3924047
Beilstein Citation (BSO):	5-26
Entry Date (DED):	1991/03/19
Update Date (DUPD):	1991/09/02

CM 1

FBRN 4014421
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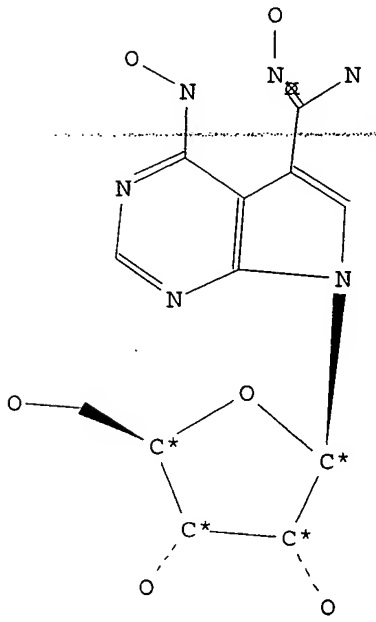

CM 2

FBRN 1098214
FMF Cl H

Field Availability:

Code	Name	Occurrence
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FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
UVS	UV and Visible Spectrum	1

This substance also occurs in Reaction Documents:

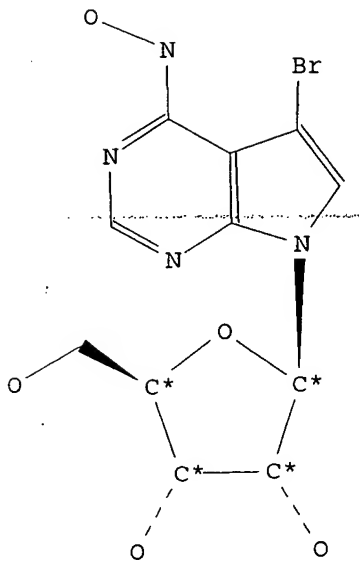
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Hinshaw et al., J.Chem.Soc.Perkin Trans.1, CODEN: JCPRB4, <1975>, 1248,1252

L12 ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN):	3628814
Beilstein Pref. RN (BPR):	24386-87-6
CAS Reg. No. (RN):	24386-87-6
Chemical Name (CN):	N6-Hydroxy-7-bromo-7-deazaadenosine
Autonom Name (AUN):	2-(5-bromo-4-hydroxyamino-pyrrolo<2,3-d>pyrimidin-7-yl)-5-hydroxymethyl-tetrahydro-furan-3,4-diol
Molec. Formula (MF):	C11 H13 Br N4 O5
Molecular Weight (MW):	361.15
Lawson Number (LN):	30366, 20554
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	3266081
Tautomer ID (TAUTID):	3525093
Beilstein Citation (BSO):	6-26
Entry Date (DED):	1991/10/23
Update Date (DUPD):	2000/03/07



Field Availability:

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CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
PHARM	Pharmacological Data	2

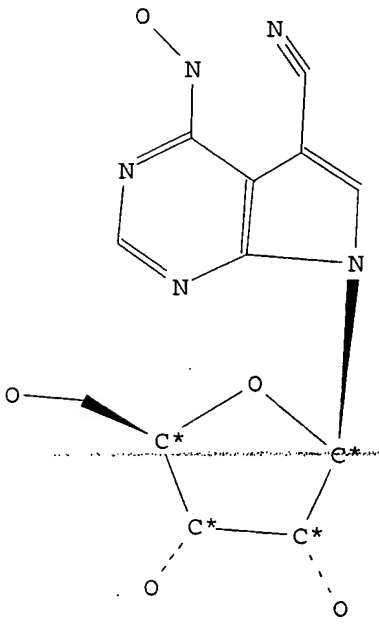
All References:
ALLREF

1. Iltzsch, Max H.; Uber, Sheri S.; Tankersley, Kevin O.; Kouni, Mahmoud H. el, Biochem.Pharmacol., CODEN: BCPCA6, 49(10), <1995>, 1501 - 1512; BABS-6185974
2. Pudlo, Jeffrey S.; Nassiri, M. Reza; Kern, Earl R.; Wotring, Linda L.; Drach, John C.; Townsend, Leroy B., J.Med.Chem., CODEN: JMCMAR, 33(7), <1990>, 1984-1992; BABS-5509325

L12 ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): 844993

Beilstein Pref. RN (BPR):	57071-72-4
CAS Reg. No. (RN):	57071-72-4
Chemical Name (CN):	4-hydroxyamino-7-β-D-ribofuranosyl-7H-pyrrolo<2,3-d>pyrimidine-5-carbonitrile
Autonom Name (AUN):	7-(3,4-dihydroxy-5-hydroxymethyl-tetrahydro-furan-2-yl)-4-hydroxyamino-7H-pyrrolo<2,3-d>pyrimidine-5-carbonitrile
Molec. Formula (MF):	C12 H13 N5 O5
Molecular Weight (MW):	307.27
Lawson Number (LN):	30367, 20554
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	811668
Tautomer ID (TAUTID):	846287
Beilstein Citation (BSO):	5-26
Entry Date (DED):	1988/11/28
Update Date (DUPD):	1992/01/31



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1

LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
UVS	UV and Visible Spectrum	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Hinshaw et al., J.Chem.Soc.Perkin Trans.1, CODEN: JCPRB4, <1975>, 1248,1252

Inventor Search

Crane 10/821,638 04/01/2005

4/4

L53 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:120918 HCAPLUS
DOCUMENT NUMBER: 142:219284
TITLE: A preparation of bicyclic imidazole derivatives, useful for the treatment of viral infections mediated by flaviviridae family of viruses
INVENTOR(S): Schmitz, Franz Ulrich; **Roberts, Christopher Don**; Griffith, Ronald Conrad; Botyanszki, Janos; Gezginci, Mikail Hakan; Gralapp, Joshua Michael; Shi, Dong Fang; Liehr, Sebastian J. R.
PATENT ASSIGNEE(S): Genelabs Technologies, Inc, USA
SOURCE: PCT Int. Appl., 327 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012288	A1	20050210	WO 2004-US24755	20040730

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-492108P P 20030801
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a preparation of bicyclic imidazole derivs. of formula I [wherein: W is CH or N; R is H, (cyclo)alkyl, alk(en/yn)yl, or (hetero)aryl, etc.; X is a fused 6,6-bicycle; Y is halogen, CN, NO2, alkyl, or acyl, etc.; Z is C(O)O-(H/alkyl/alk(en/yn)yl), C(O)NH(alkyl), or C(O)NH(aryl), etc.], useful for the treatment of viral infections mediated by flaviviridae family of viruses. For instance, benzimidazole derivative II (HCV-NS5b enzyme assay, inhibition data: at 100 μM - 98.22%, at 33 μM - 92.74%) was prepared via amidation of III by aminoacid IV with a yield of 32% (example 4).
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1080873 HCAPLUS
DOCUMENT NUMBER: 142:56309
TITLE: Preparation of substituted imidazole derivatives as antiviral agents
INVENTOR(S): **Roberts, Christopher Don**; Shi, Dong-Fang;

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004028481	A2	20040408	WO 2003-US31433	20030930
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004147464	A1	20040729	US 2003-676956	20030930
PRIORITY APPLN. INFO.:			US 2002-415222P P	20020930
			US 2003-443169P P	20030129

OTHER SOURCE(S): MARPAT 140:327061

AB Nucleoside compns. and methods for treating **hepatitis** C virus infections. Thus, 9-(2'-C-methyl-β-D-ribofuranosyl)-6-methoxyaminopurine was prepared by the reaction of 6-chloro-9-(2'-C-methyl-β-D-ribofuranosyl)purine and methxylamine. This compound exhibited anti-**hepatitis** C activity by inhibiting HCV polymerase.

L53 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:226373 HCAPLUS

TITLE: Designing an enriched screening library for the discovery of non-nucleoside inhibitors of the HCV NS5b RNA polymerase

AUTHOR(S): Schmitz, Uli; Kirk, Martin; Fung, Kevin; McCoy, Samantha Koo; Latour, Derek; Michelotti, Emil; Pouliot, Jeff; Dunlop, Kevin; **Roberts, Christopher**; Lou, Lillian; Griffith, Ronald

CORPORATE SOURCE: Genelabs Technologies, Inc, Redwood City, CA, 94063, USA

SOURCE: Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, United States, March 28-April 1, 2004 (2004), MEDI-015. American Chemical Society: Washington, D. C.
CODEN: 69FGKM

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB **Hepatitis** C is considered a major public health threat and current therapies still call for major improvements. The virus causing **Hepatitis** C (HCV) is a single-stranded RNA virus, whose replication in liver cells relies on several virally-encoded nonstructural proteins, including the NS5b RNA-dependent RNA polymerase. To date, a few non-nucleoside inhibitors have been published, but the wide range of inhibitors for HIV reverse transcriptase, a functionally and structurally closely related polymerase, are largely inactive against HCV NS5b. Recognizing that kinases and RNA polymerases have a common substrate, ATP, one would expect that a compound collection enriched with the chemotypes found among a plethora of kinase inhibitors should have a higher hit-rate against the NS5b polymerase compared to a diverse random library of the same size. Based on chemotypes found in .apprx.50 diverse kinase and ATPase inhibitors found in the literature, we selected over 30,000 compds. from one particular com. source and subjected them to a rigorous diversity pruning step. Our final HTS library indeed produced a hit rate of 0.88 %

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004063658	A1	20040401	US 2003-431631	20030506
EP 1501850	A2	20050202	EP 2003-747674	20030506

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

PRIORITY APPLN. INFO.:	US 2002-378624P	P	20020506
	US 2002-392871P	P	20020628
	WO 2003-US14237	W	20030506

OTHER SOURCE(S): MARPAT 139:365176

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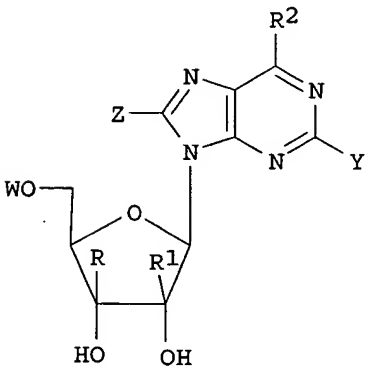

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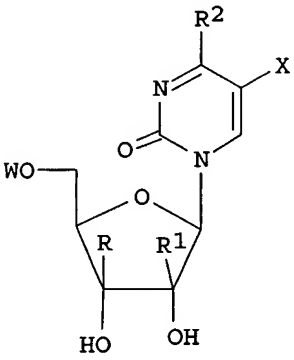

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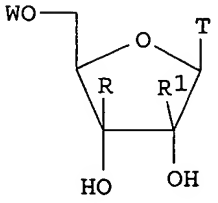


III

AB Nucleosides I-III, wherein R and R1 are independently H, alkyl, alkenyl, alkynyl, provided that R and R1 are not both H; R2 is alkyl, cycloalkyl, alkenyl, alkynyl, acylamino, guanidino, amidino, thioacylamino, OH, alkoxy, halo, nitro, aryl, heteroaryl, substituted amine; W is H, phosphate, phosphonate, acyl, alkyl, sulfonate, lipid, amino acid, sugar residue, peptide, cholesterol; X is H, halo, alkyl, substituted amine; Y is H, halo, OH, alkylthio, substituted amine; Z is H, halo, OH, alkyl, substituted amine; T is nucleobase, were prepared as HCV RNA polymerase inhibitors and for treating **hepatitis** C virus infections. Thus, 2-(4-amino-pyrrolo[3,2-c]pyridin-1-yl)-5-hydroxymethyl-3-methyltetrahydro-

AB Compds. of formula R1Z1COX1NHCOX2CONHX3COZ2R2 [wherein Z1 and Z2 = independently NR3, O; R3 = H, alkyl; R1 and R2 = independently substituted alkyl or aryl, (un)substituted heteroaryl; X2 = (un)substituted aryl or heteroaryl, alkenyl, alkynyl, cycloalkyl, heterocyclic; X1 and X3 = independently (un)substituted aryl or heteroaryl, CHR4; R4 = (un)natural amino acid side chain; or their pharmaceutically acceptable salts] were prepared as topoisomerase inhibitors (no data) for use as antibacterial, antifungal, and/or antitumor agents. For example, 1H-indole-2,5-dicarboxylic acid dipentafluorophenyl ester was reacted with at least two equivalent of 4-amino-1-methyl-1H-pyrrole-2-carboxylic acid [2-(carbamimidoyl)ethyl]amide in DMF to give I. Compds. of the invention exhibited antibacterial and antifungal activity with some having minimal inhibitory concns. of <45.5 μM. DNA binding assays showed that invention compds. bind to DNA very tightly, with apparent Kd,app values below 100 nM for most compds. tested.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:27216 HCAPLUS

DOCUMENT NUMBER: 136:241074

TITLE: Minor groove DNA binders as antimicrobial agents. 1. Pyrrole tetraamides are potent antibacterials against vancomycin resistant enterococci and methicillin resistant Staphylococcus aureus

AUTHOR(S): **Dyatkina, Natalia B.**; **Roberts, Christopher D.**; Keicher, Jesse D.; Dai, Yuqin; Nadherny, Joshua P.; Zhang, Wentao; Schmitz, Uli; Kongpachith, Ana; Fung, Kevin; Novikov, Alexander A.; Lou, Lillian; Velligan, Mark; Khorlin, Alexander A.; Chen, Ming S.

CORPORATE SOURCE: Genelabs Technologies, Redwood City, CA, 94063, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(4), 805-817
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

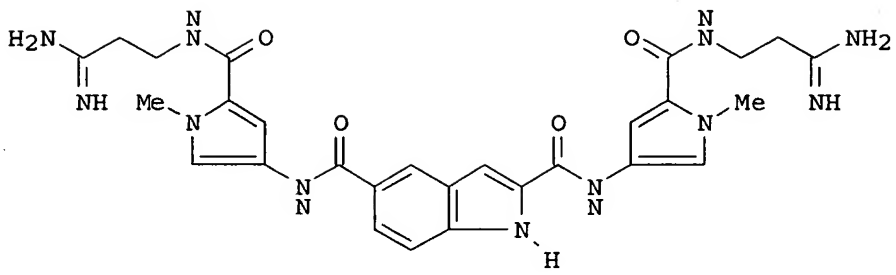
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:241074

AB A new series of short pyrrole tetraamides are described whose submicromolar DNA binding affinity is an essential component for their strong antibacterial activity. This class of compds. is related to the linked bis-netropsins and bis-distamycins, but here, only one amino-pyrrole-carboxamide unit and an amidine tail is connected to either side of a central dicarboxylic acid linker. The highest degree of DNA binding, measured by compound-induced changes in UV melting temps. of an AT-rich DNA oligomer, was observed for flat, aromatic linkers with no inherent bent, i.e., terephthalic acid or 1,4-pyridine-dicarboxylic acid. However, the antibacterial activity is critically linked to the size of the N-alkyl substituent of the pyrrole unit. None of the tetraamides with the commonly used methyl-pyrrole showed antibacterial activity. Isoamyl- or cyclopropylmethylene-substituted dipyrrole derivs. have the min. inhibitory concns. in the submicromolar range. In vitro toxicity against human T-cells was studied for all compds. The degree to which compds. inhibited cell growth was neither directly correlated to DNA binding affinity nor directly correlated to antibacterial activity but seemed to depend strongly on the nature of the N-alkyl pyrrole substituents.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



I

AB Compds. of formula R1Z1COX1NHCOX2CONHX3COZ2R2 (Z1 and Z2 = independently NR3, O; R3 = H, alkyl; R1 and R2 = independently substituted alkyl or aryl, (un)substituted heteroaryl; X2 = (un)substituted aryl or heteroaryl, alkenyl, alkynyl, cycloalkyl, heterocyclic; X1 and X3 = independently (un)substituted aryl or heteroaryl, CHR4; R4 = (un)natural amino acid side chain) or their pharmaceutically acceptable salts were prepared and possess one or more of the following activities: antibacterial, antifungal and antitumor activity. For example, 1H-Indole-2,5-dicarboxylic acid dipentafluorophenyl ester was reacted with at least two equivalent of 4-amino-1-methyl-1H-pyrrole-2-carboxylic acid (2-carbamimidoyl-ethyl)-amide in DMF to give compound I. Compds. of this invention exhibited antibacterial and antifungal activity with some having minimal inhibitory concns. of <45.5 μM. Studies of their DNA binding properties demonstrated that they bind to DNA very tightly, with apparent Kd,app values below 100 nM for most compds. tested.